Scalable Multigrid Methods Using Fortran90 and MPI

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Outline

- Multigrid algorithms for implicit dynamics
- Element level parallelism
- Nested mesh generation and partitioning
- Algorithm performance
- Application to ASCI coupled solid rocket simulations
- Extensions to adaptive mesh refinement
- Future developments

Nonlinear Implicit Dynamics

Loop over time:

Loop over Newton iterations:

Solve

$$\left(\frac{1}{\beta\Delta t^2}\boldsymbol{M}+\boldsymbol{K}_T^{(k)}\right)\Delta\boldsymbol{u}^{(k)}=\boldsymbol{f}_{t+\Delta t}-\boldsymbol{i}_{t+\Delta t}^{(k)}-\frac{1}{\beta\Delta t^2}\boldsymbol{M}\boldsymbol{u}_{t+\Delta t}^{(k)}+\frac{1}{\beta\Delta t^2}\boldsymbol{M}\boldsymbol{u}_t+\frac{1}{\beta\Delta t}\boldsymbol{M}\dot{\boldsymbol{u}}_t+\boldsymbol{M}\ddot{\boldsymbol{u}}_t$$

Increment displacements

$$\boldsymbol{u}_{t+\Delta t}^{(k+1)}=\boldsymbol{u}_{t+\Delta t}^{(k)}+\Delta\boldsymbol{u}^{(k)}$$

End loop over Newton iterations

Compute velocities and accelerations

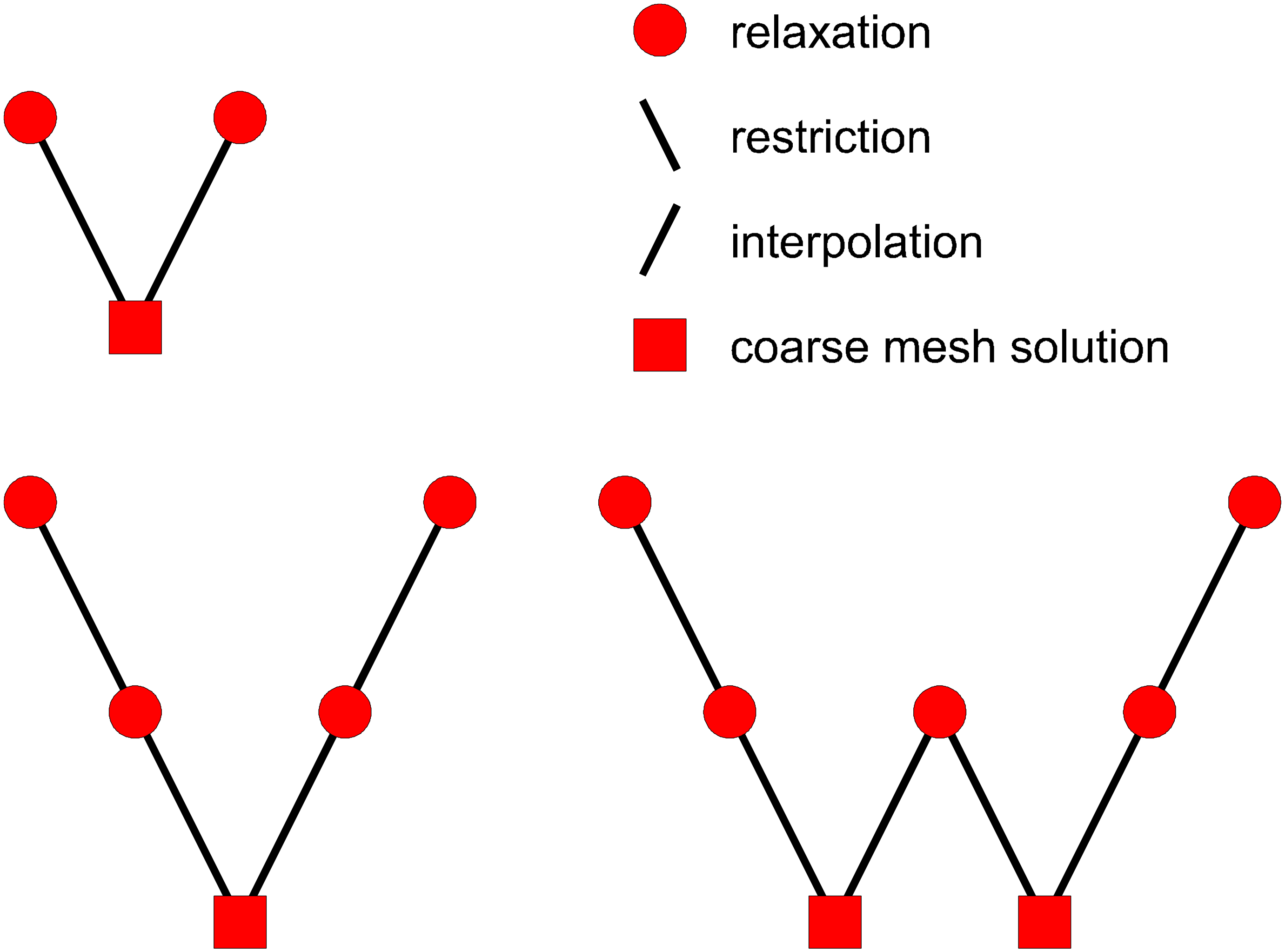
$$\ddot{\boldsymbol{u}}_{t+\Delta t}=\frac{1}{\beta\Delta t^2}\left(\boldsymbol{u}_{t+\Delta t}-\boldsymbol{u}_t\right)-\frac{1}{\beta\Delta t}\dot{\boldsymbol{u}}_t-\ddot{\boldsymbol{u}}_t$$

$$\dot{\boldsymbol{u}}_{t+\Delta t}=\dot{\boldsymbol{u}}_t+\frac{\Delta t}{2}\left(\ddot{\boldsymbol{u}}_t+\ddot{\boldsymbol{u}}_{t+\Delta t}\right)$$

End loop over time

Parallel Multigrid Methods

- Use multigrid to solve linear matrix equations in nonlinear algorithms
- Basic two grid method
  - iterative methods quickly produce a smooth error on a fine mesh
  - compute the smooth error on a coarse mesh
- Recursion produces multigrid method
- Computational effort is linearly proportional to problem size (algorithmically scalable)
- Element level parallelism gives scalable performance


relaxation
restriction
interpolation
coarse mesh solution

Multigrid Components

- **Relaxation**
  - **Jacobi, Gauss-Seidel perform poorly for ill-conditioned problems**
  - **preconditioned conjugate gradient**
- **Interpolation, restriction**
  - **nodal averaging for nested meshes**
- **Coarse mesh solution**
  - **compute coarse mesh matrix from coarse mesh elements**
  - **preconditioned conjugate gradient**

PCG Relaxation

Given $\quad \boldsymbol{x}^{(0)}, \; l = 0$

Initialize
$$\boldsymbol{r}^{(0)} = \boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}^{(0)}$$
$$\boldsymbol{d}^{(0)} = \boldsymbol{A}_D^{-1}\boldsymbol{r}^{(0)}$$
$$\boldsymbol{p}^{(0)} = \boldsymbol{d}^{(0)}$$

Iterate
$$\alpha^{(l)} = \frac{\left\langle \boldsymbol{r}^{(l)}, \boldsymbol{d}^{(l)} \right\rangle}{\left\langle \boldsymbol{p}^{(l)}, \boldsymbol{A}\boldsymbol{p}^{(l)} \right\rangle}$$
$$\boldsymbol{x}^{(l+1)} = \boldsymbol{x}^{(l)} + \alpha^{(l)}\boldsymbol{p}^{(l)}$$
$$\boldsymbol{r}^{(l+1)} = \boldsymbol{r}^{(l)} - \alpha^{(l)}\boldsymbol{A}\boldsymbol{p}^{(l)}$$
$$\boldsymbol{d}^{(l+1)} = \boldsymbol{A}_D^{-1}\boldsymbol{r}^{(l+1)}$$
$$\beta^{(l+1)} = \frac{\left\langle \boldsymbol{r}^{(l+1)}, \boldsymbol{d}^{(l+1)} \right\rangle}{\left\langle \boldsymbol{r}^{(l)}, \boldsymbol{d}^{(l)} \right\rangle}$$
$$\boldsymbol{p}^{(l+1)} = \boldsymbol{d}^{(l+1)} + \beta^{(l+1)}\boldsymbol{p}^{(l)}$$
$$l = l + 1$$

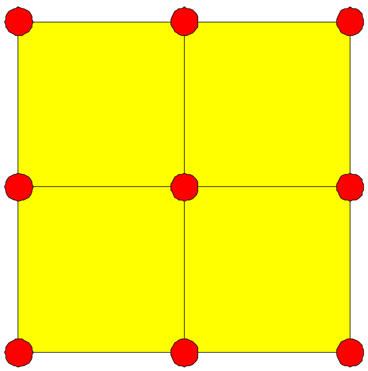
Primary operations

- matrix-vector multiplications $\boldsymbol{A}\boldsymbol{p}^{(l)}$
- DAXPYs $\quad \boldsymbol{p}^{(l+1)} = \boldsymbol{d}^{(l+1)} + \beta^{(l+1)}\boldsymbol{p}^{(l)}$
- scalar products $\left\langle \boldsymbol{p}^{(l)}, \boldsymbol{A}\boldsymbol{p}^{(l)} \right\rangle$
- preconditioning $\quad \boldsymbol{d}^{(l+1)} = \boldsymbol{A}_D^{-1}\boldsymbol{r}^{(l+1)}$

Intergrid Transfer Operators

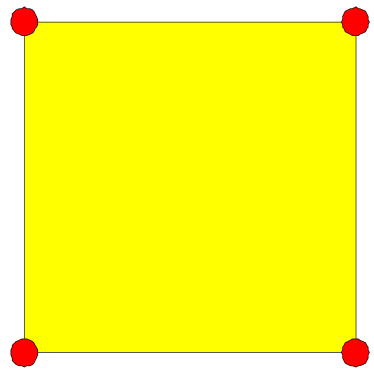
Fine mesh

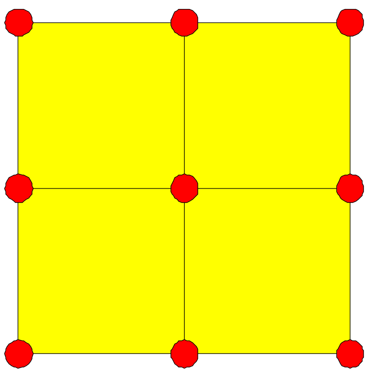
Coarse mesh



$$\Delta \boldsymbol{x}_f^{(k)} = \boldsymbol{I}_c^f \Delta \boldsymbol{x}_c^{(k)}$$

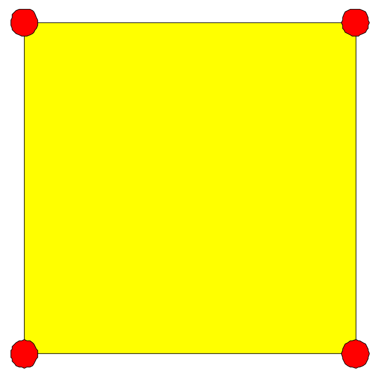
$$\boldsymbol{I}_c^f = \boldsymbol{T}$$





$$\boldsymbol{r}_c^{(k)} = \boldsymbol{I}_f^c \boldsymbol{r}_f^{(k)}$$

$$\boldsymbol{I}_f^c = \boldsymbol{T}^T$$



Primary operations

matrix-vector multiplications

$$\boldsymbol{r}_c^{(k)} = \boldsymbol{T}^T \boldsymbol{r}_f^{(k)}$$

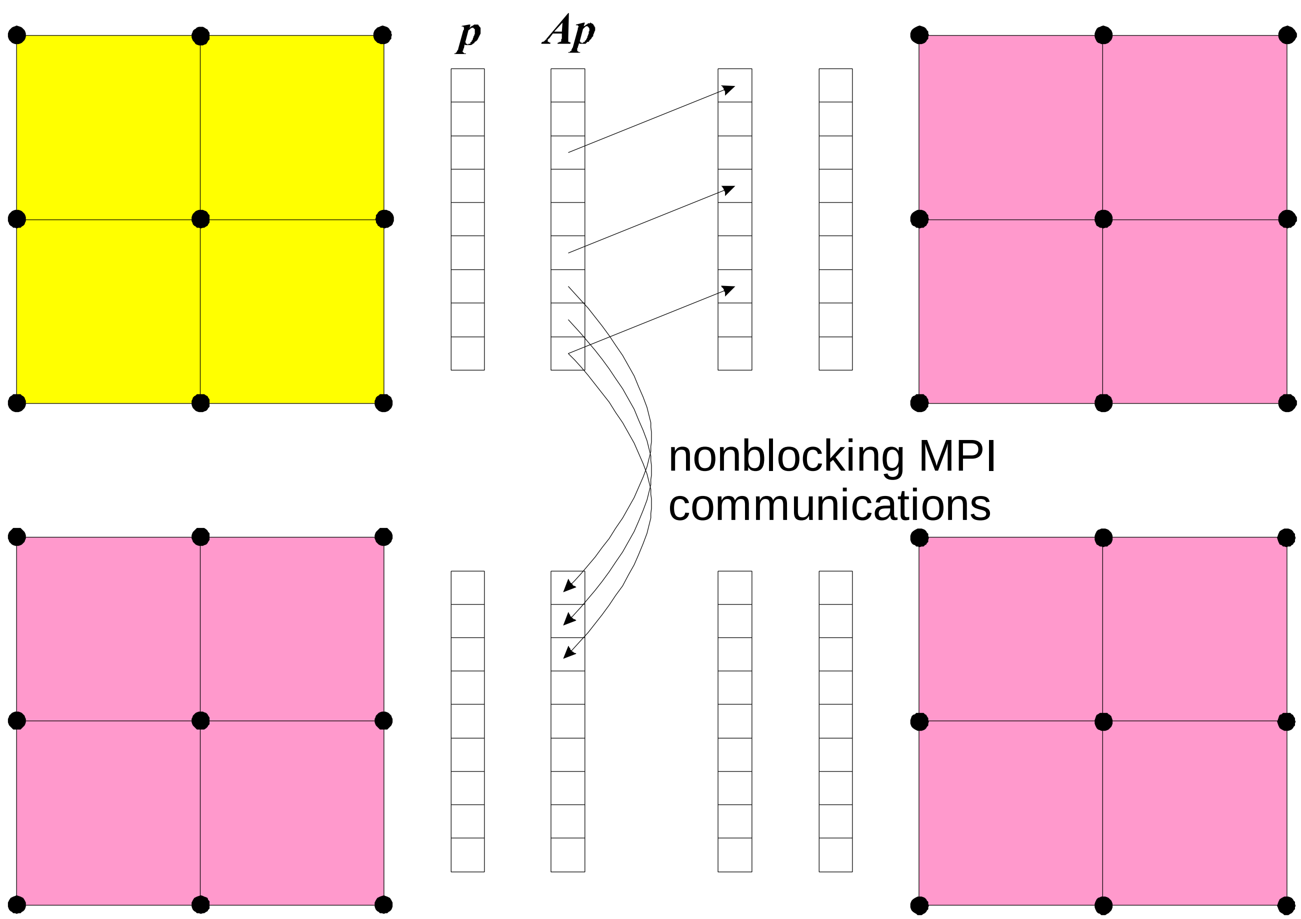
$$\Delta \boldsymbol{x}_f^{(k)} = \boldsymbol{T} \Delta \boldsymbol{x}_c^{(k)}$$

Element Level Computations

- **All operations can be performed independently on partitioned domains**
- **Interprocessor communications required during**
  - **matrix-vector multiplications**
  - **scalar products**
  - **fine to coarse mesh restriction**
- **Matrix-free computations reduce storage and CPU time**

$$\boldsymbol{K}\boldsymbol{p} = \sum_e \boldsymbol{K}^e \boldsymbol{p}^e = \sum_e \left(\int_{\Re^e} \boldsymbol{B}^T \boldsymbol{D}\boldsymbol{B} \, dV \right) \boldsymbol{p}^e$$

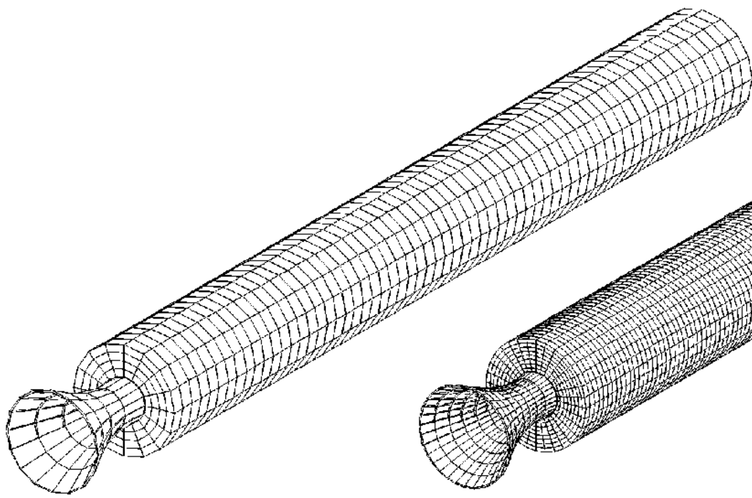
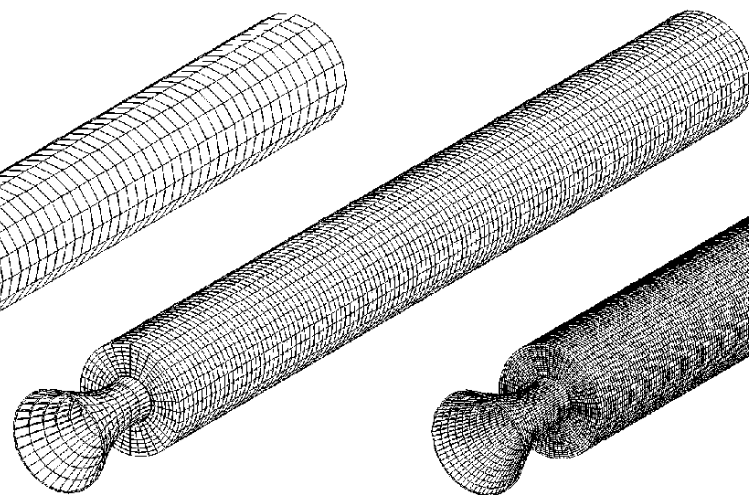
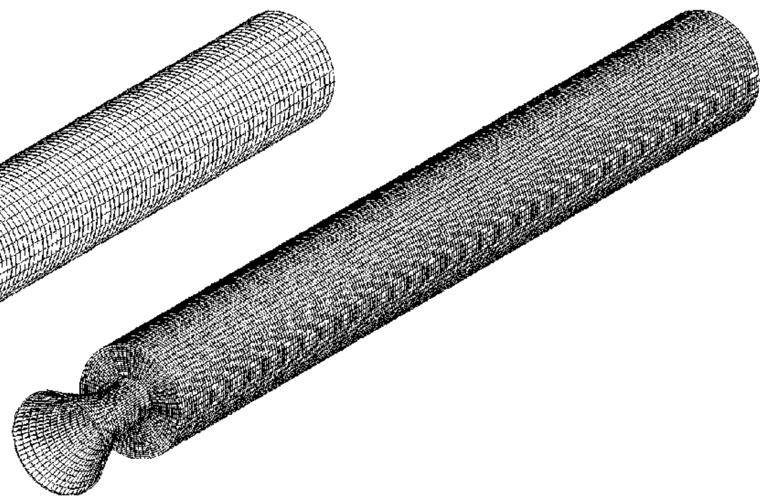
Distributed Memory Implementation



Mesh Generation

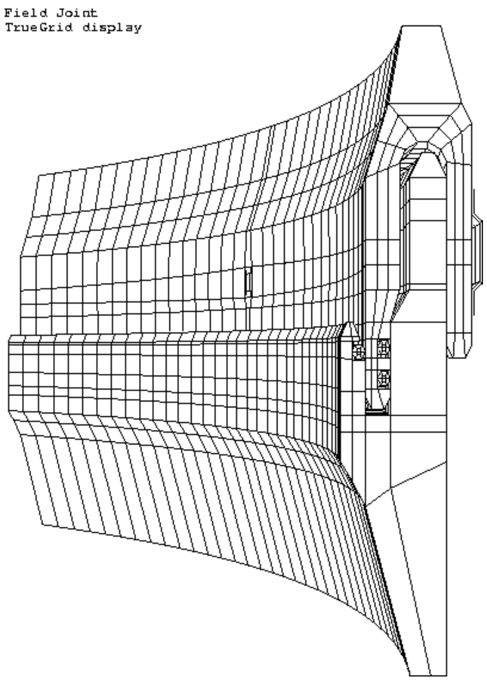
- Multigrid requires a hierarchy of increasingly finer meshes
- Adaptive mesh refinement will eventually be used to generate this hierarchy
- *Truegrid* is employed to produce a sequence of nested, uniformly refined hexahedral meshes
- Complex parts can be modeled in this manner

Solid Rocket Motor

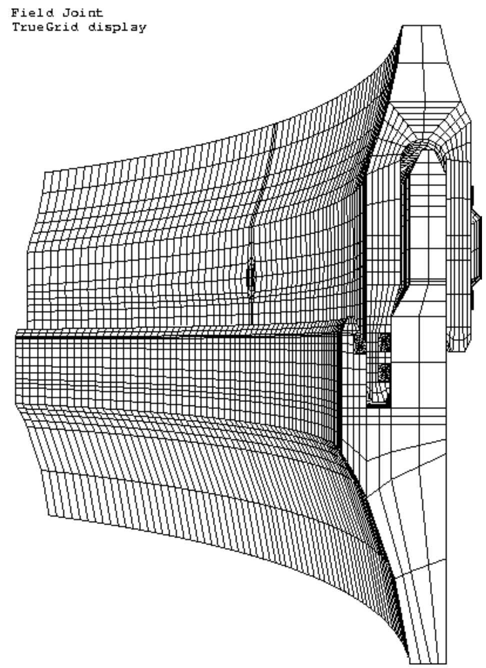




4,096 32,768 262,144

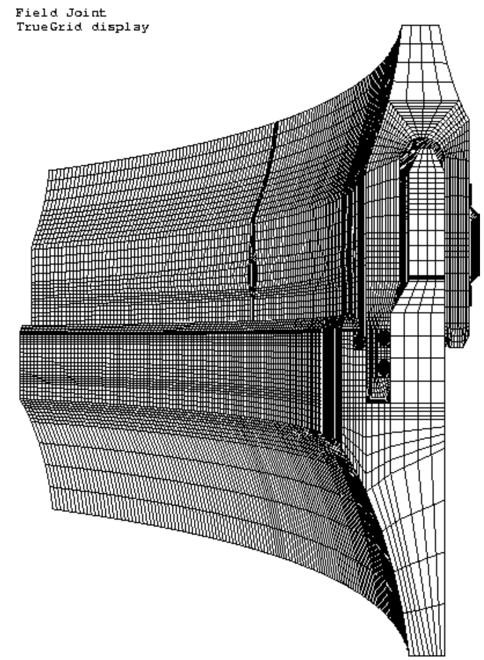
Rocket Joint Detail



3,624



28,992

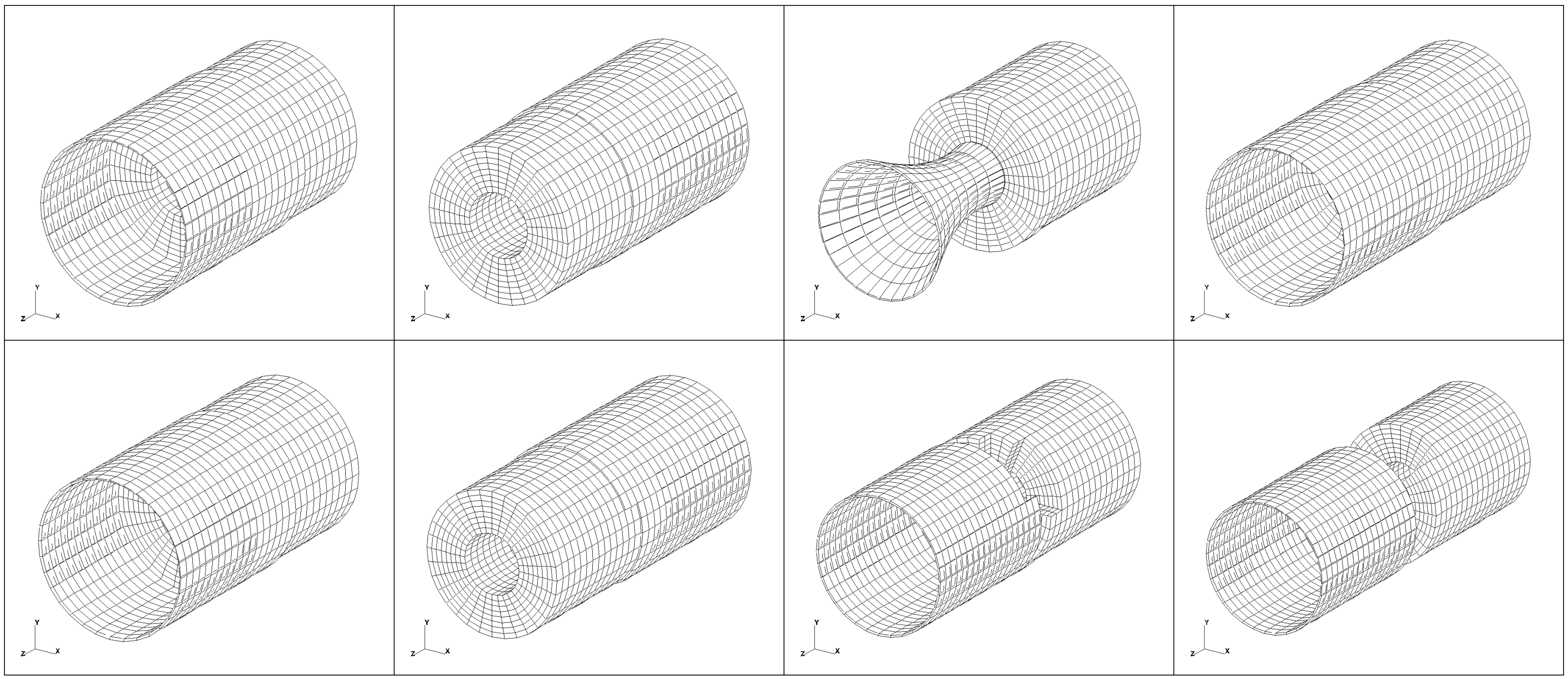


231,936

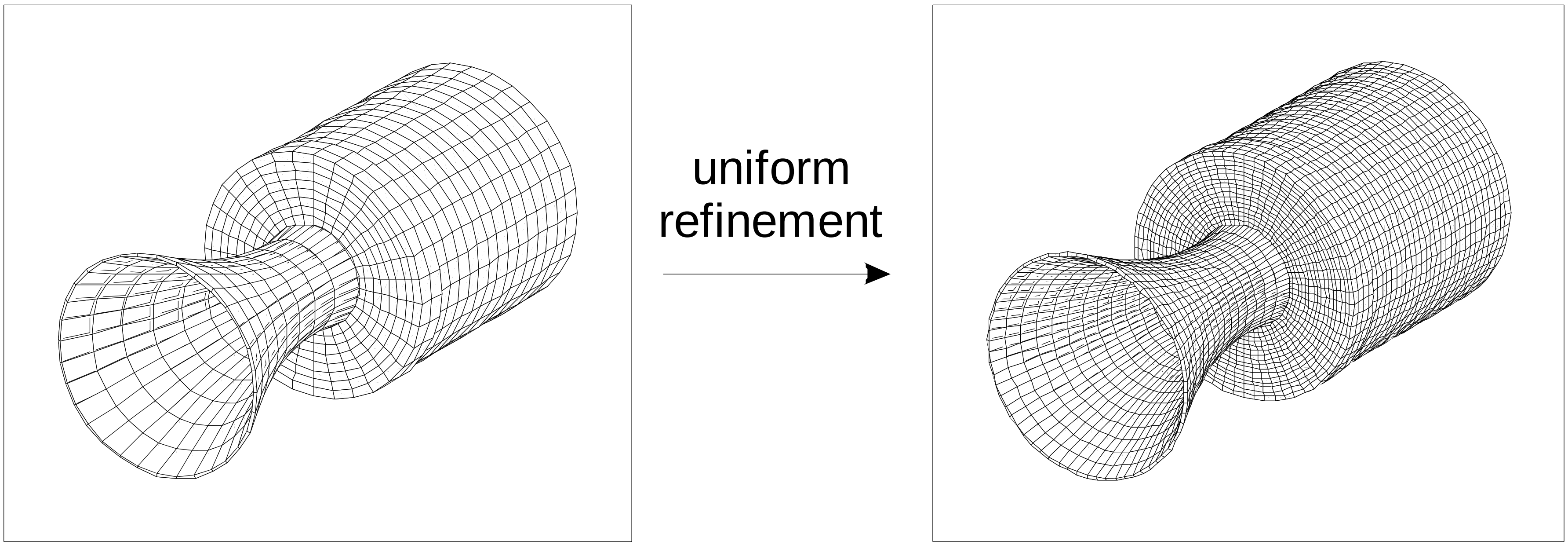
Mesh Partitioning

- Partitioning is performed on the coarsest mesh using *Metis* to achieve perfect load balance
- Uniform refinement of the coarsest mesh partitions produces partitions on all of the fine meshes
- Perfect element load balance is maintained throughout the mesh hierarchy
- Communications may not be optimum

Coarsest Mesh Partitions



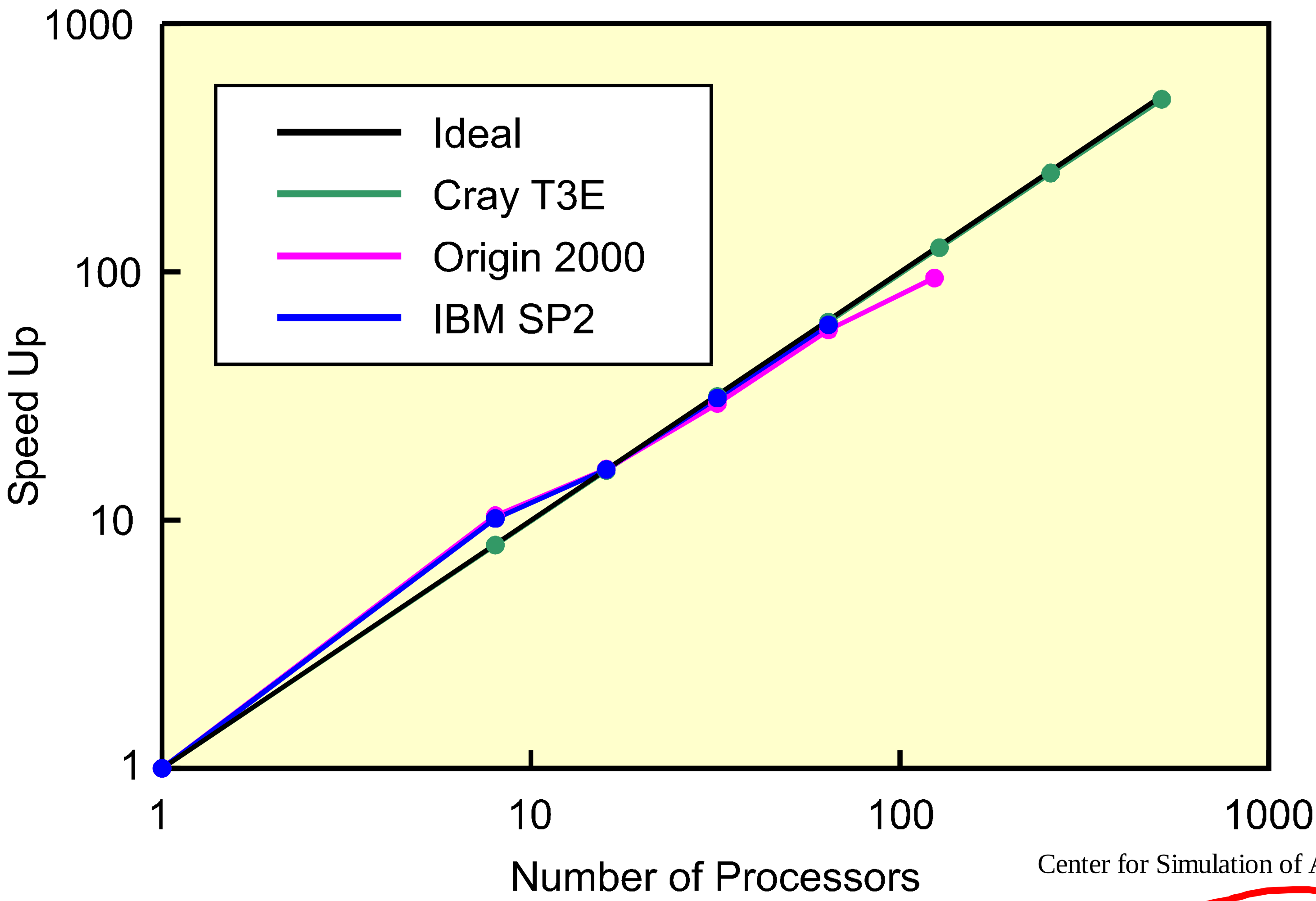
Partition Mesh Refinement



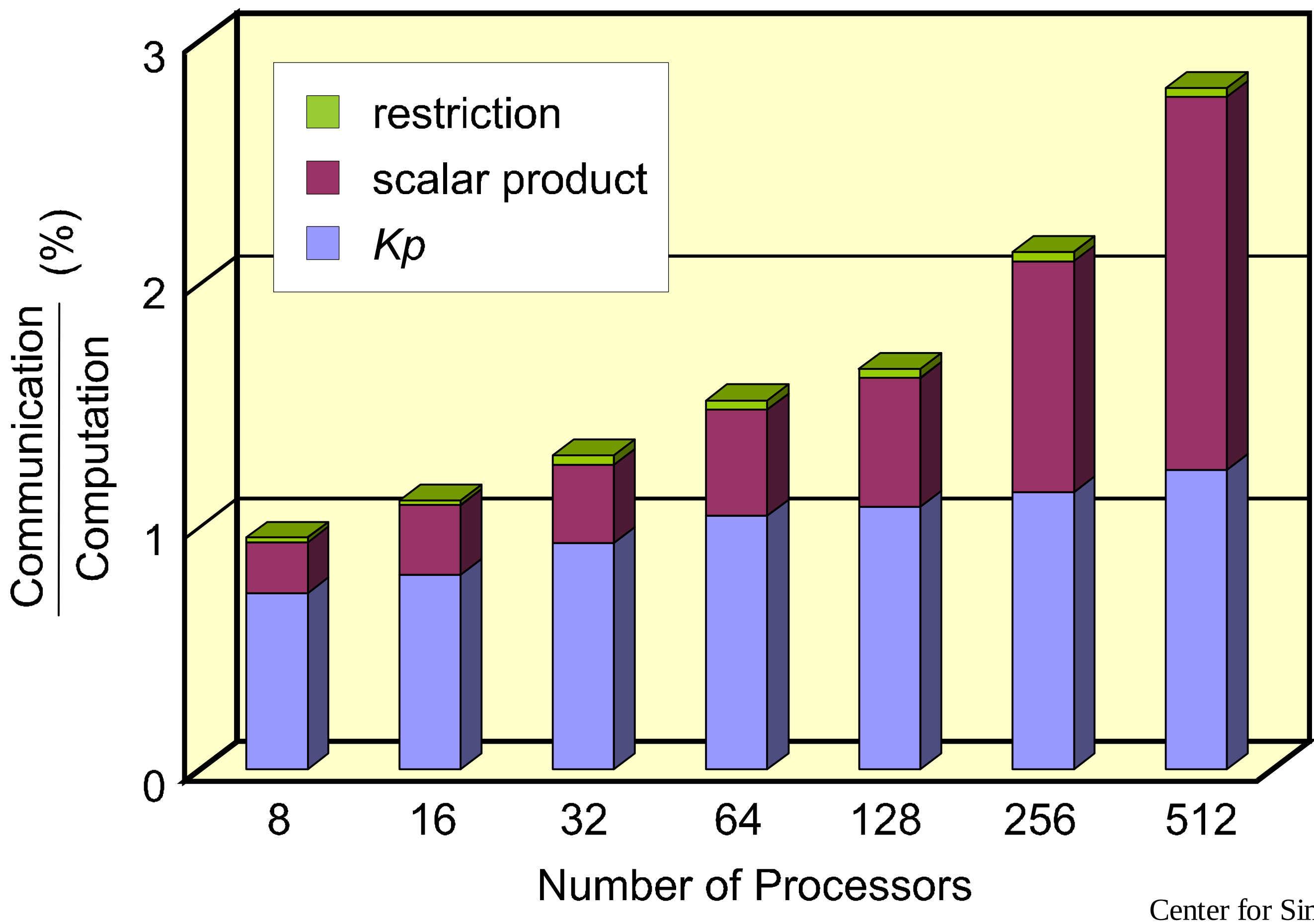
Parallel Performance

- Code has been benchmarked on several multiprocessor machines
  - IBM SP2 (Argonne)
  - SGI Origin 2000 (NCSA)
  - SGI Cray T3E (PSC)
- Computation dominates communication
- Scalable element computations
- Cray T3E showed the best performance
- Lazy processors on Origin 2000

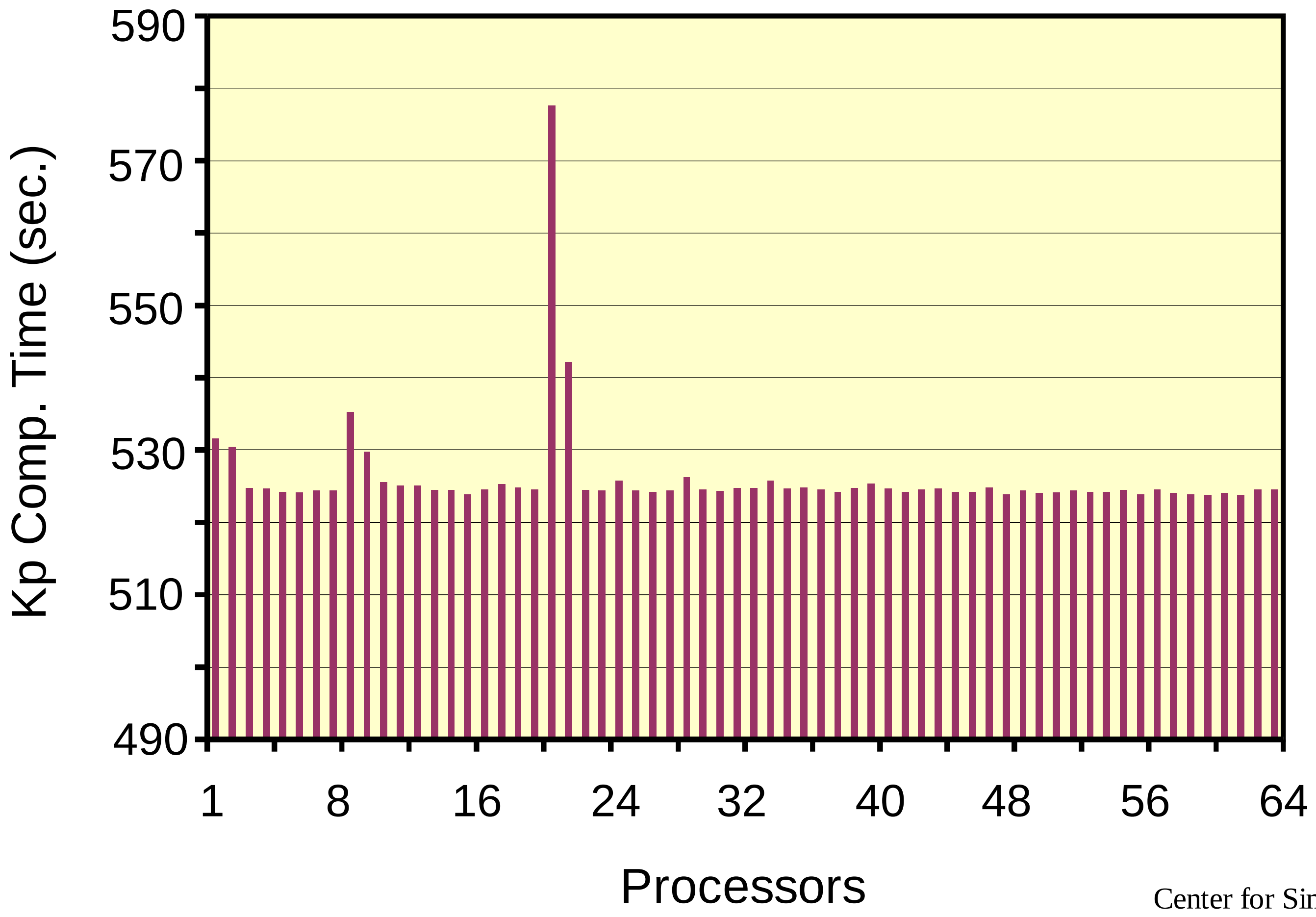
Scalability Results



Cray T3E Cost Analysis



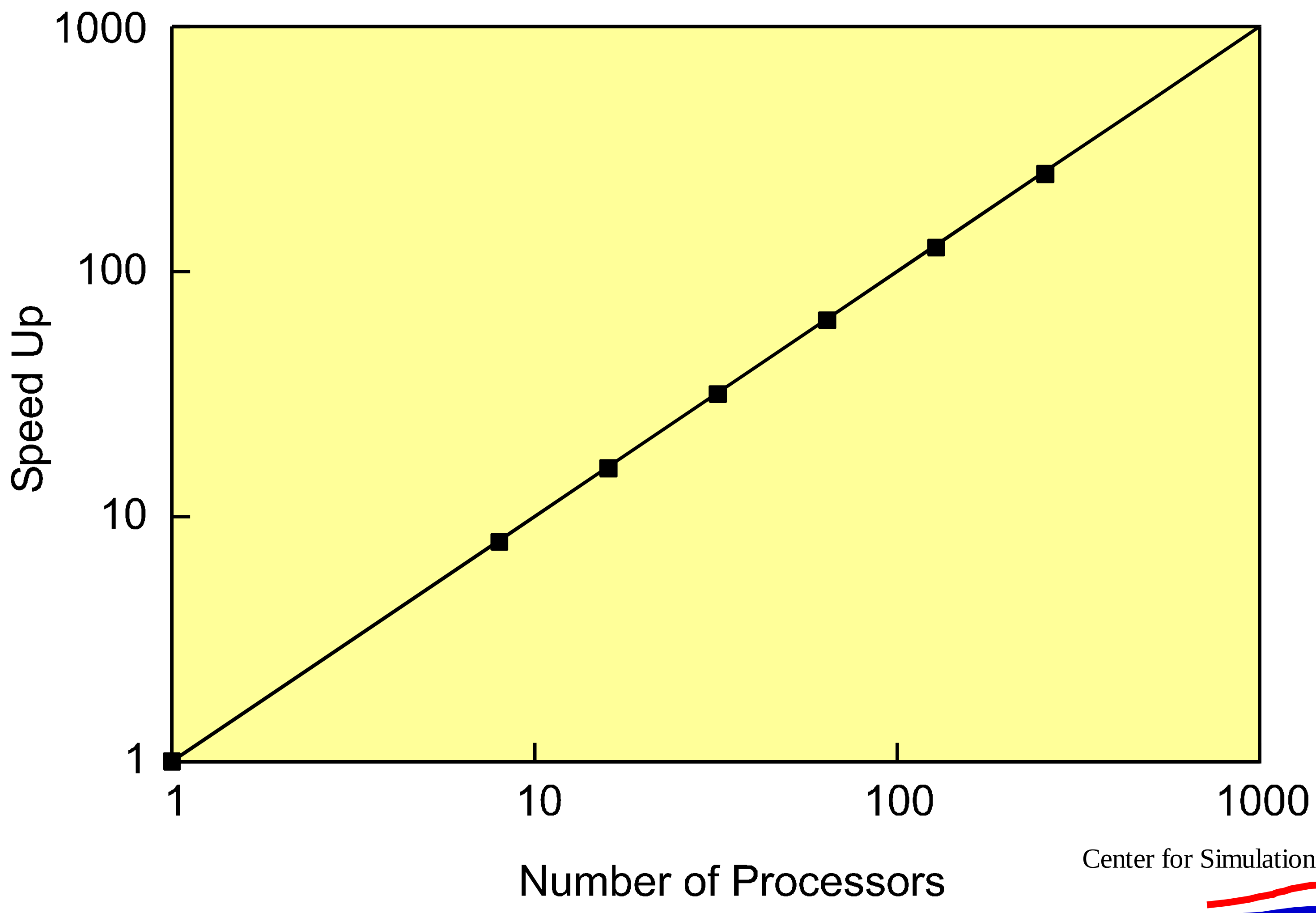
Origin 2000 Performance



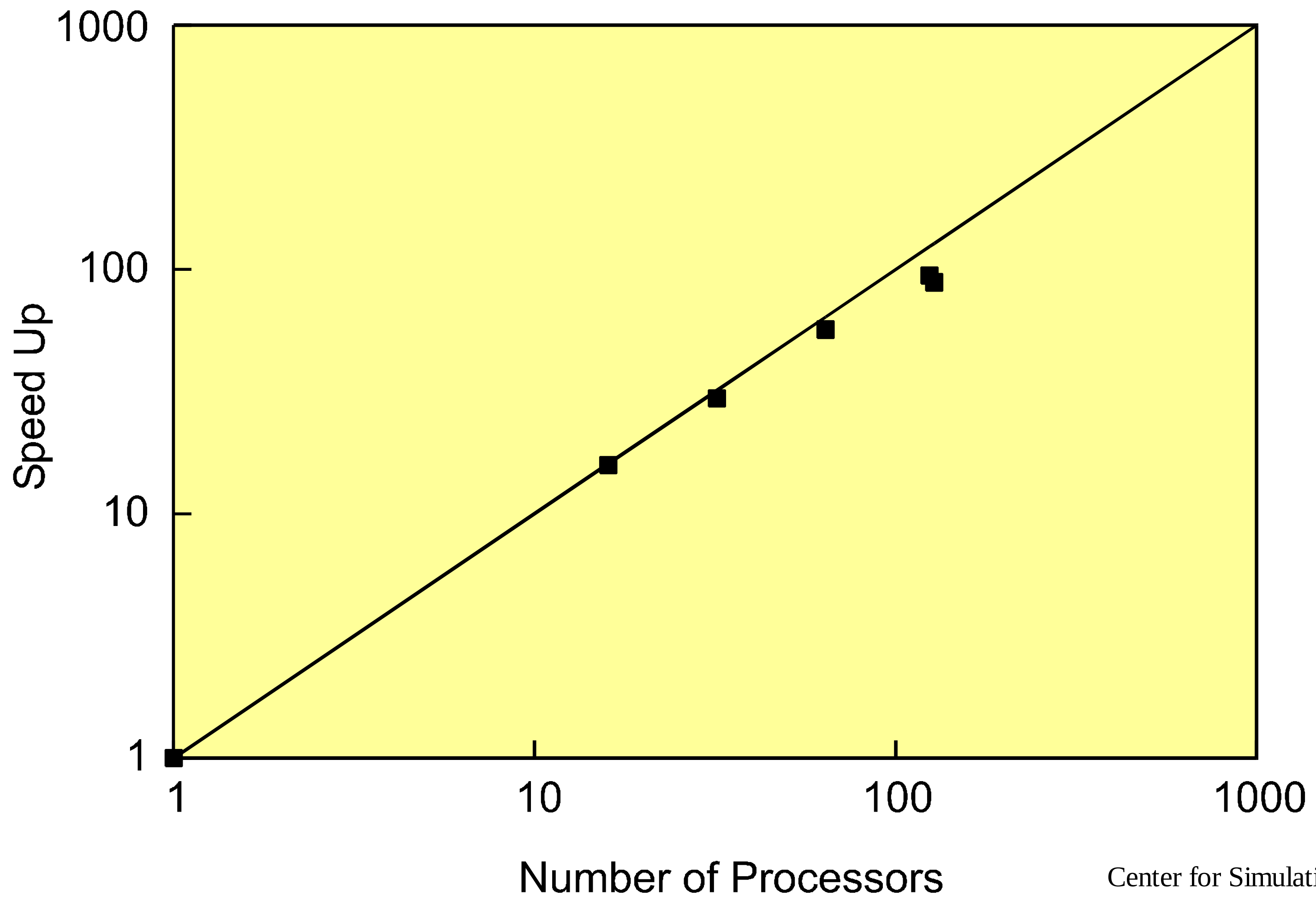
Coupled Solid Rocket Simulations

- **ROCSOLID**
  - **unstructured finite elements**
  - **implicit time integrator**
  - **multigrid equation solver**
- **ROCFLO**
  - **unsteady 3D, compressible Navier-Stokes equations on dynamic meshes**
  - **structured finite volumes**
  - **explicit time integrator**
- **Combustion model**
  - ***ap^n* used as interface regression rate**
- **Interface conditions**
  - **specify b.c.'s for each module**

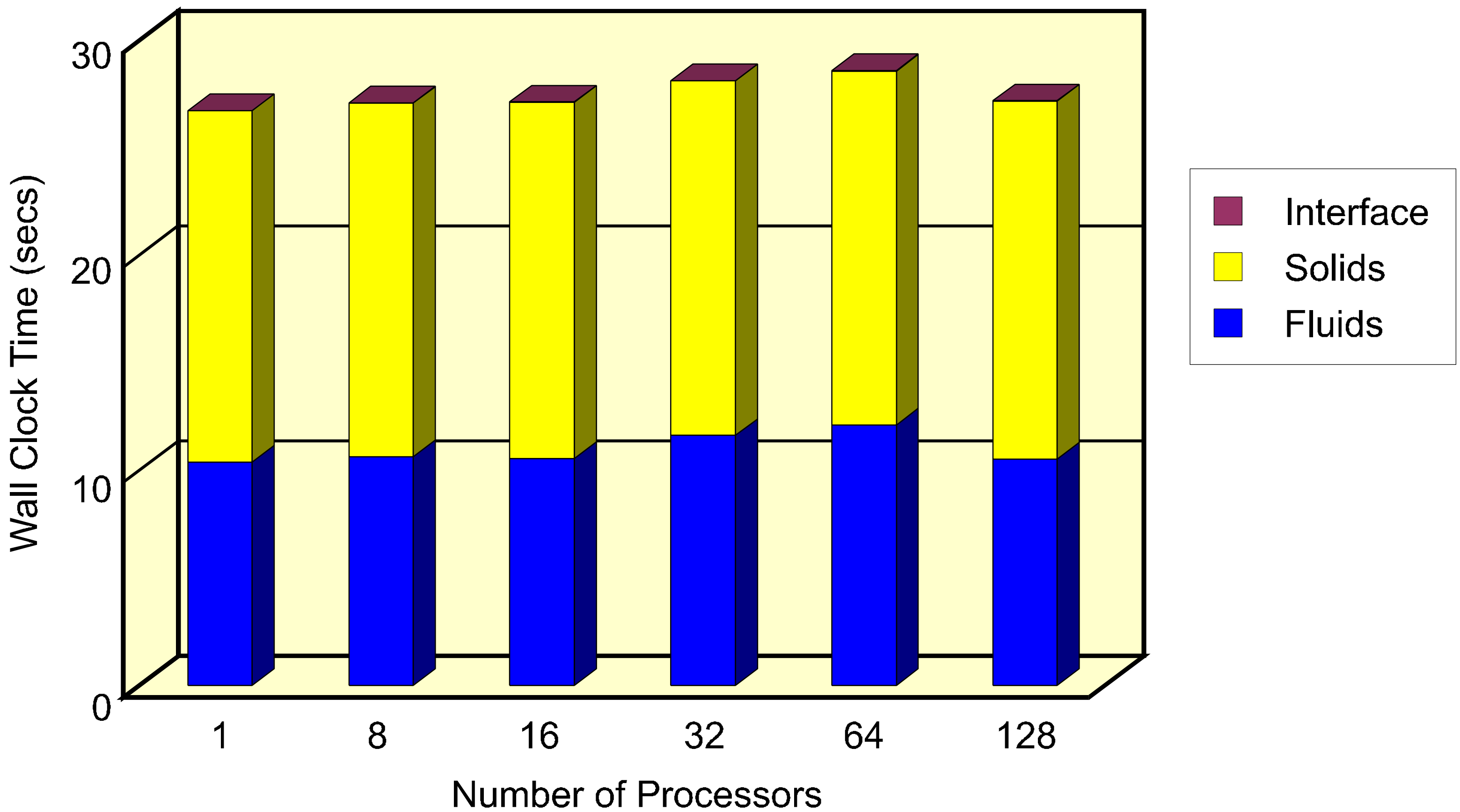
Cray T3E Scalability Results



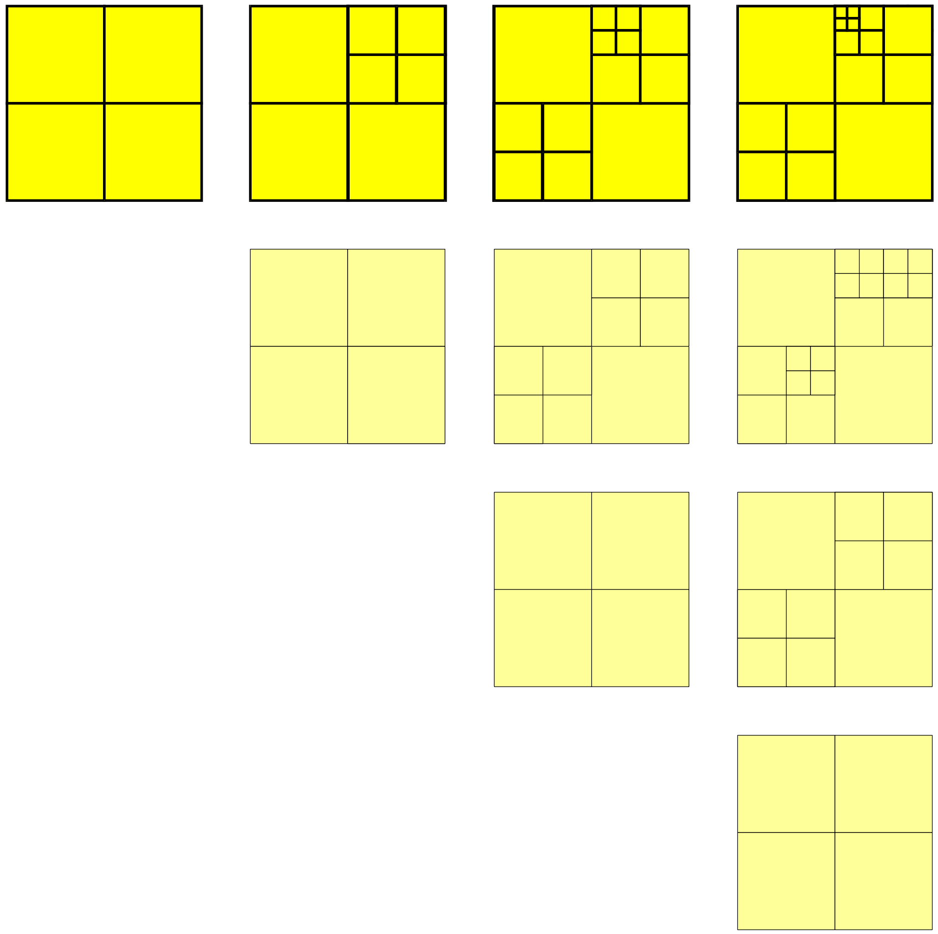
Origin 2000 Scalability Results

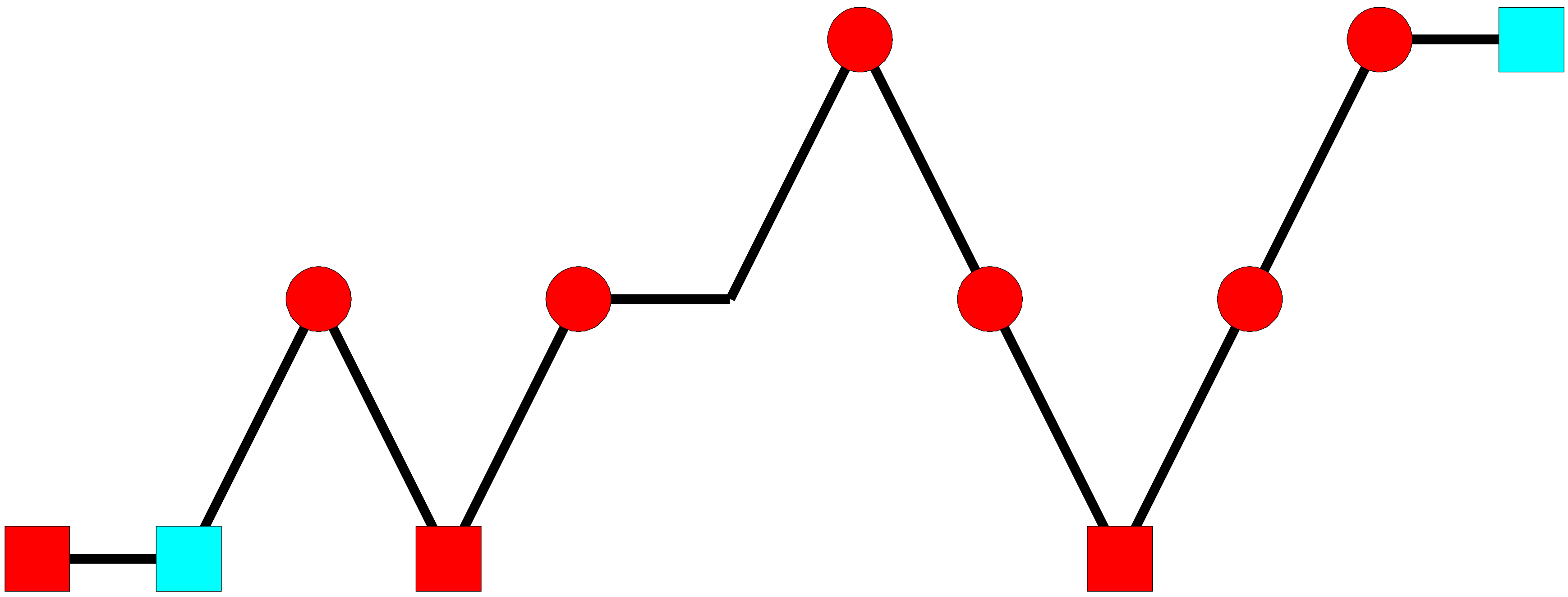


GEN1 T3E Time Requirements

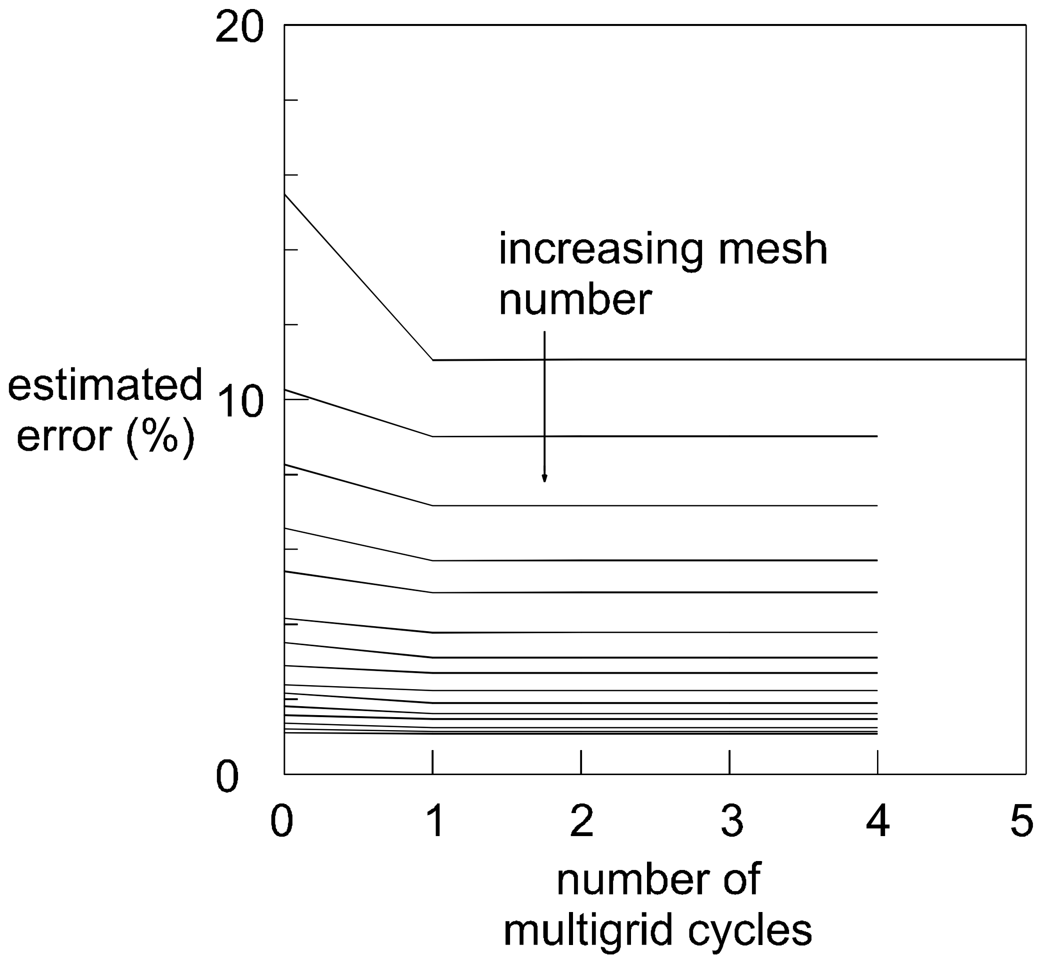


Adaptive Meshing and Multigrid

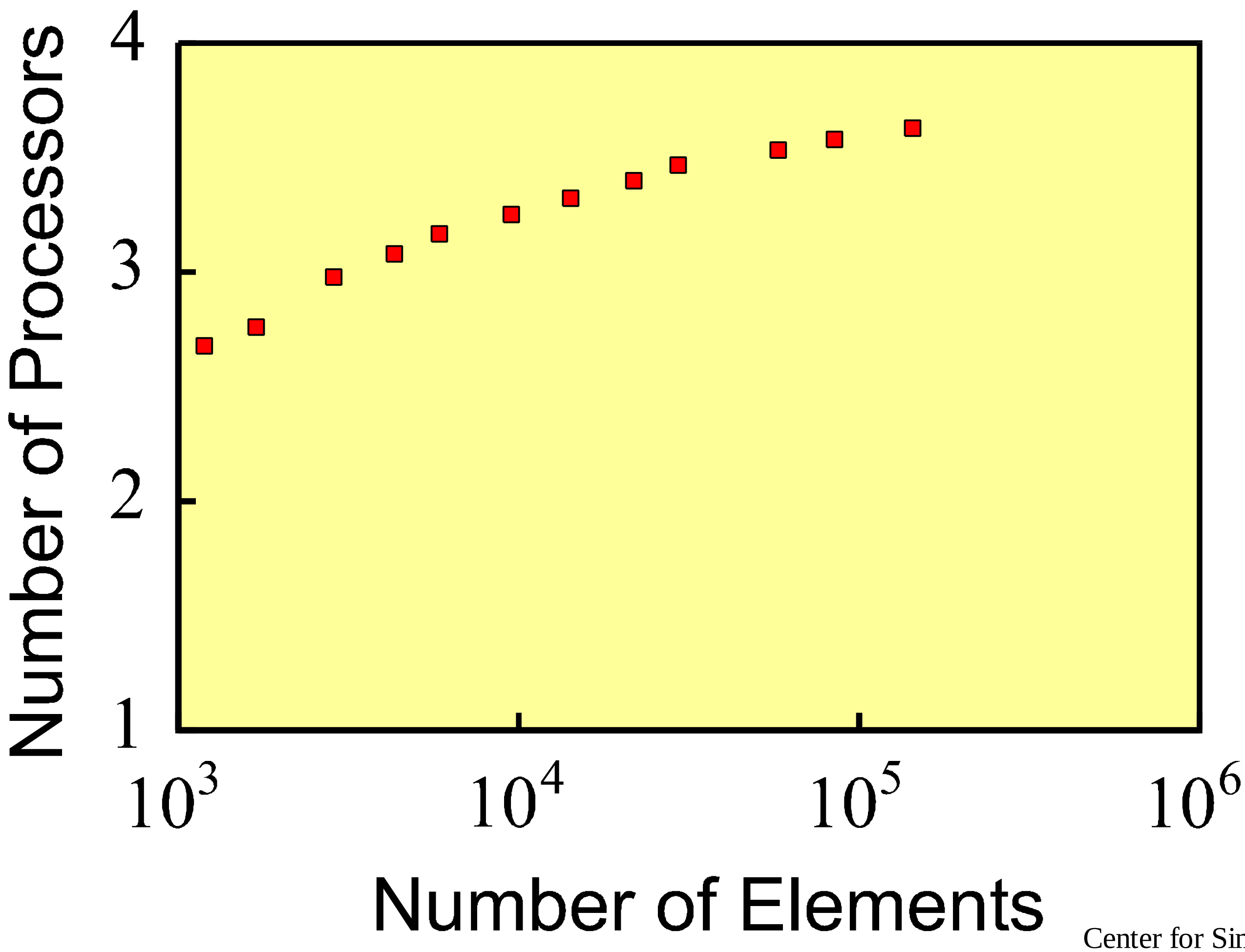




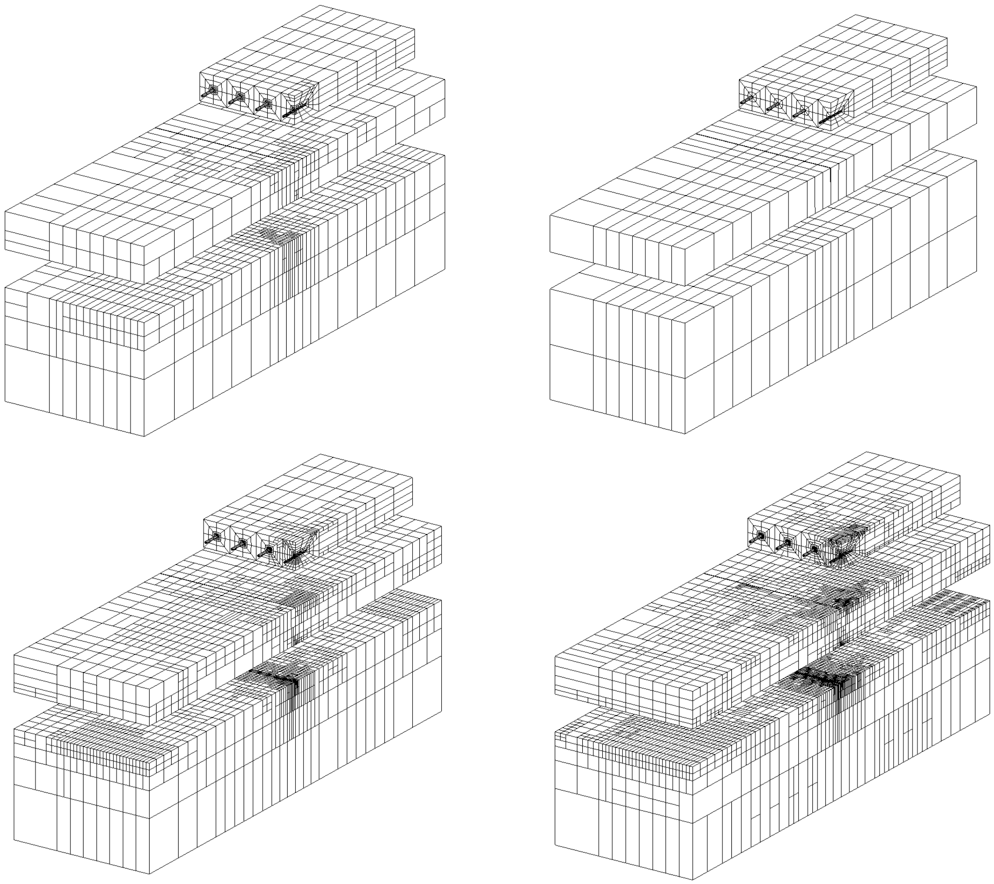
AMR-MG Convergence

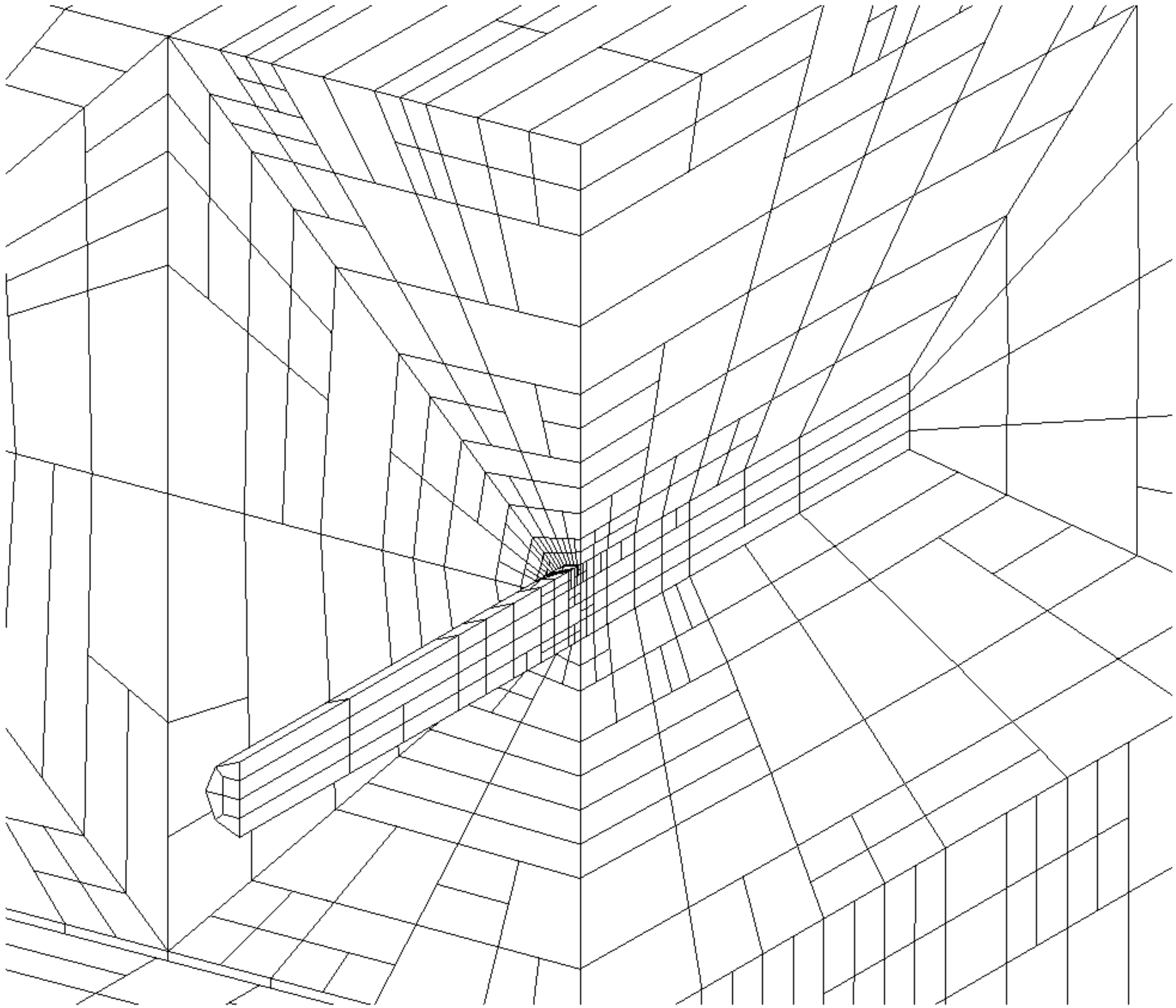


AMR-MG Parallel Speed-Up



AMR-MG Meshes





Future Plans

- **Shells using enhanced assumed strain solid elements**
- **Advanced material models**
- **Scalable nonsymmetric solvers for ALE**
- **Parallel contact algorithms**
- **Adaptive mesh refinement and shared memory parallelism**
- **Integration into Charm++ environment for AMR-MG in a distributed memory environment**

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